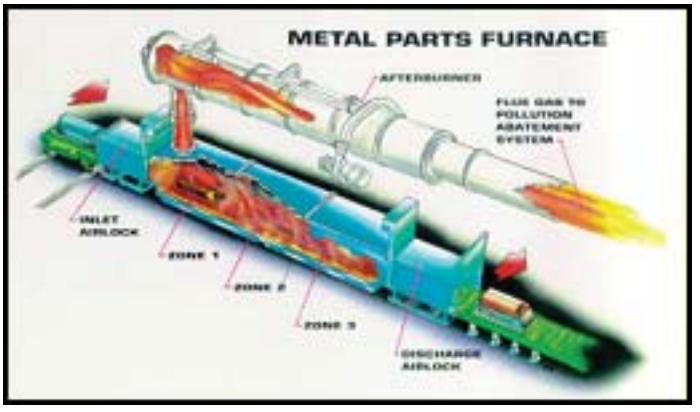
Chemical Demilitarization Simulations



Incineration is one of the technologies used by the U.S. Army to destroy the highly toxic chemical agents and munitions contained within the Chemical Weapons Stockpile. Reaction Engineering International (REI) is developing advanced computer simulation tools for analyzing chemical demilitarization incinerators. These tools integrate the range of models and visualization methods that are required to perform simulations to analyze the performance and emissions from military incinerator units under a broad range of operating conditions and configurations for different munitions and storage containers. The simulation workbench developed a tightly integrated problem solving process, with plug and play functionality, designed for use by non-specialists, and provides the capability to interrogate a simulation at multiple levels of detail in a seamless manner. The simulations provide the researcher with detailed information on the local gas properties, such as gas temperature, species concentrations (e.g., oxygen, agent, combustion products, products of incomplete combustion), and pressure. Likewise, the models also provide detailed information on the surface temperatures and heat fluxes to the furnace walls and munitions within the incinerator. This information is used to develop a deeper level of understanding of the combustion process, agent destruction, and product species concentrations when processing munitions or equipment contaminated by GB, VX and mustard gas. The models also provide the ability to study a wide range of "what if" scenarios for both standard and emergency incinerator operation.

Phase III IMPACTS

- $337K in sales to DoD
- $98.5K in sales to U.S. EPA- National Homeland Security Research Center
- Models for chemical agent decomposition contained in the Incinerator Simulator used to convince regulators to allow chemical weapons incineration plant to resume full operation after an agent detect incident. Resulting long term operating cost savings to the chemical weapons program estimated to be in excess of $1B.
- Incinerator Simulator being used in U.S. Army Chemical Materials Agency (CMA) Risk Issue Matrix (RIM) project with Washington Group International (WGI) to evaluate processing of undrained mustard projectiles in Metal Parts Furnace.
- Incinerator Simulator being tailored for use by EPA and National Homeland Security Research Center to investigate methods to incinerate building materials contaminated with agents from a chemical or biological terrorist attack on an office building.